

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016681.D
 Acq On : 02 Oct 2021 21:21
 Operator : CG/JU
 Sample : M3829-24
 Misc :
 ALS Vial : 49 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 RE123D2-20210918

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016681.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	28	rVB	12897	30545	8.76%	1.024%
2	3.816	76	80	86	rBV	14086	42397	12.15%	1.422%
3	3.908	86	90	105	rVB	105811	348807	100.00%	11.697%
4	4.821	185	189	203	rVB	47607	109759	31.47%	3.681%
5	5.263	234	237	247	rVB	8350	21895	6.28%	0.734%
6	5.678	279	282	297	rVB2	2717	11116	3.19%	0.373%
7	6.647	383	387	401	rVB	4251	10968	3.14%	0.368%
8	6.822	403	406	419	rVB	6185	17754	5.09%	0.595%
9	7.264	449	454	460	rBV	9799	22404	6.42%	0.751%
10	7.633	490	494	500	rVB	52103	108416	31.08%	3.636%
11	7.864	515	519	525	rBV	11768	24060	6.90%	0.807%
12	8.168	549	552	560	rVV	7124	20249	5.81%	0.679%
13	8.306	564	567	569	rVB	10865	13553	3.89%	0.454%
14	8.784	601	605	610	rBV	27431	56020	16.06%	1.879%
15	10.191	713	716	729	rBV	149674	258956	74.24%	8.684%
16	10.407	729	733	736	rBV	109526	190084	54.50%	6.374%
17	12.003	920	931	942	rBV	51569	84869	24.33%	2.846%
18	12.886	1071	1074	1078	rBV	103971	174533	50.04%	5.853%
19	13.178	1094	1097	1107	rBV	49771	81912	23.48%	2.747%
20	14.269	1180	1183	1186	rBV	140534	201262	57.70%	6.749%
21	14.434	1193	1196	1201	rBV	5109	9141	2.62%	0.307%
22	15.017	1239	1242	1246	rBV	6038	9672	2.77%	0.324%
23	15.715	1294	1297	1299	rBV	8146	11839	3.39%	0.397%
24	15.766	1299	1301	1307	rVB2	10169	16796	4.82%	0.563%
25	17.018	1400	1403	1406	rBV	106908	163843	46.97%	5.494%
26	18.909	1661	1665	1681	rVB	22334	26409	7.57%	0.886%
27	19.063	1687	1696	1721	rBV	154413	218900	62.76%	7.341%
28	19.674	1813	1819	1841	rBV	133297	174110	49.92%	5.839%
29	21.164	1992	1995	1998	rBV	26403	32871	9.42%	1.102%
30	21.227	1998	2001	2010	rVV	133728	197947	56.75%	6.638%
31	22.321	2100	2104	2109	rBV	3630	7595	2.18%	0.255%
32	22.841	2231	2239	2251	rVB	5055	7846	2.25%	0.263%
33	23.419	2399	2408	2415	rBV	8169	13760	3.94%	0.461%
34	23.481	2415	2426	2475	rVB	101347	209081	59.94%	7.011%
35	24.087	2592	2603	2630	rBV	7994	16735	4.80%	0.561%
36	24.854	2815	2827	2852	rBV2	7868	18930	5.43%	0.635%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	25.754	3071	3090	3121	rBV	2312	7221	2.07%	0.242%
38	26.818	3382	3401	3425	rBV	1785	6244	1.79%	0.209%
39	28.085	3750	3771	3792	rBV2	957	3538	1.01%	0.119%

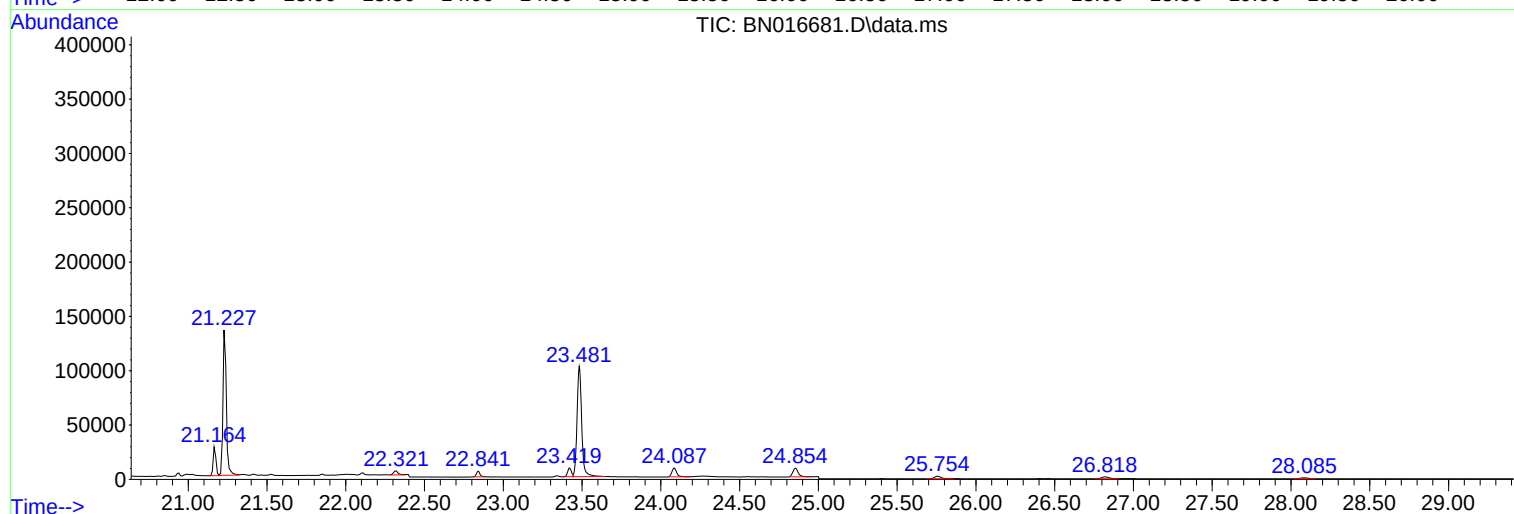
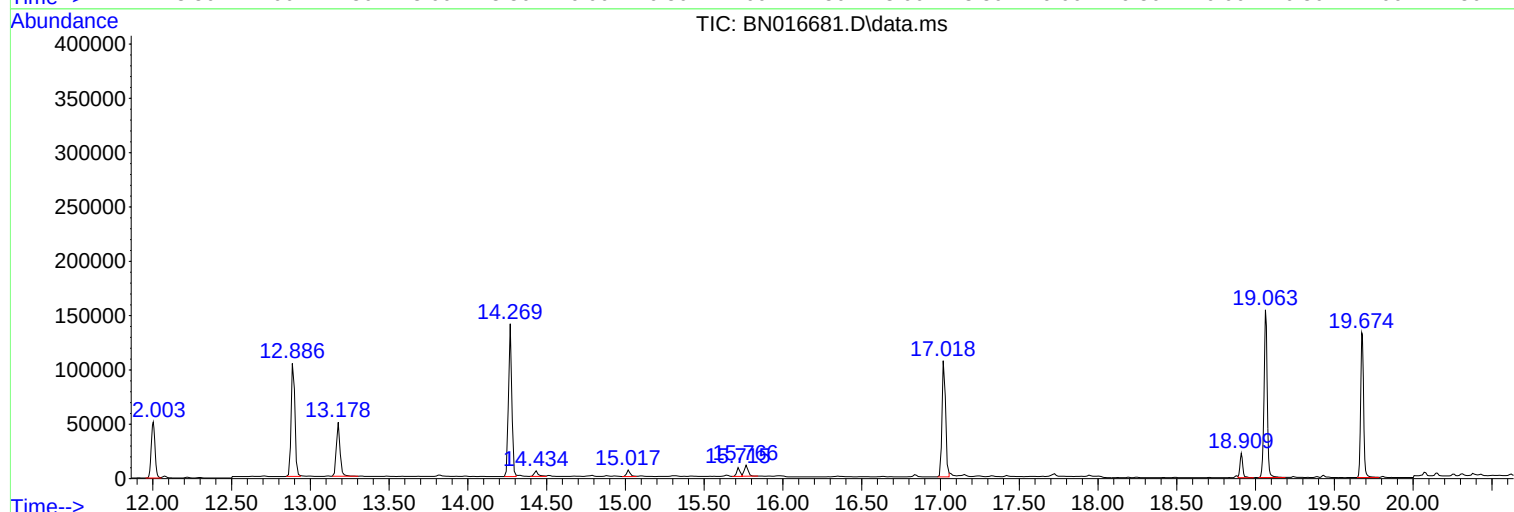
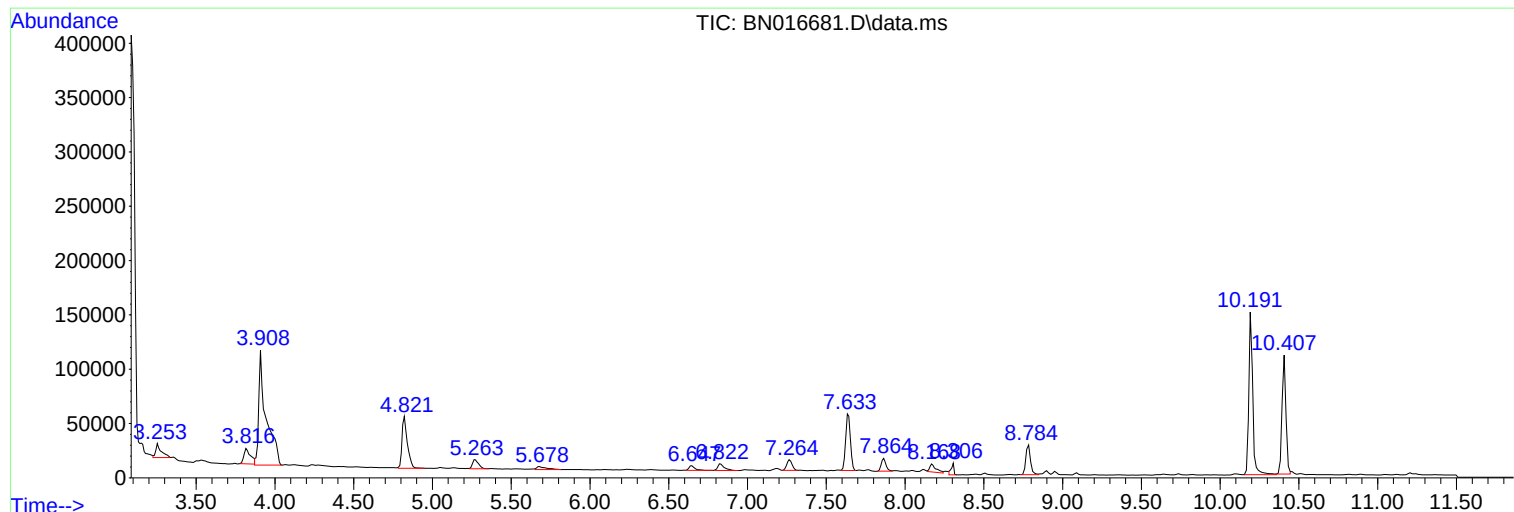
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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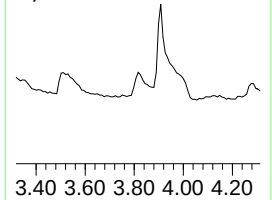
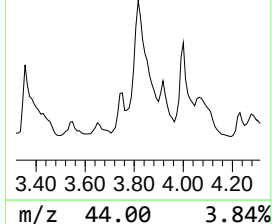
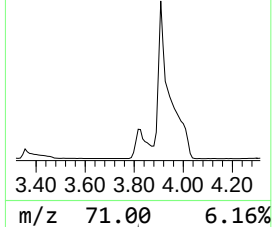
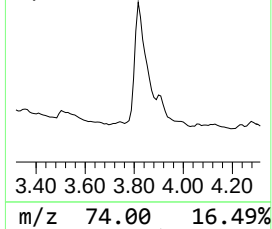
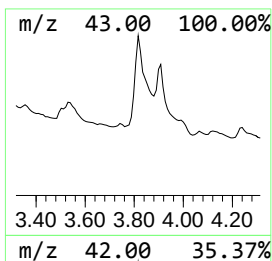
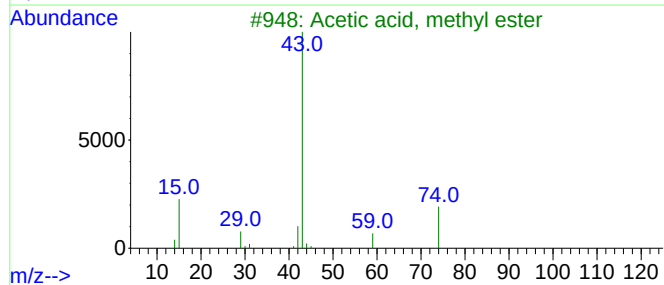
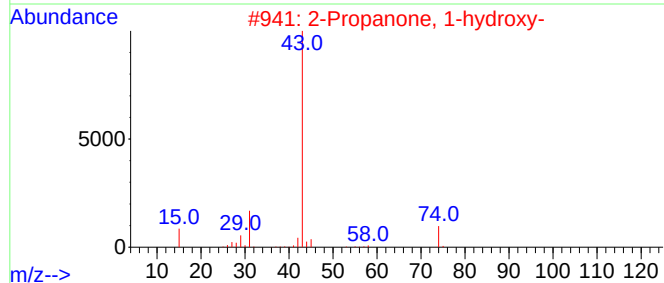
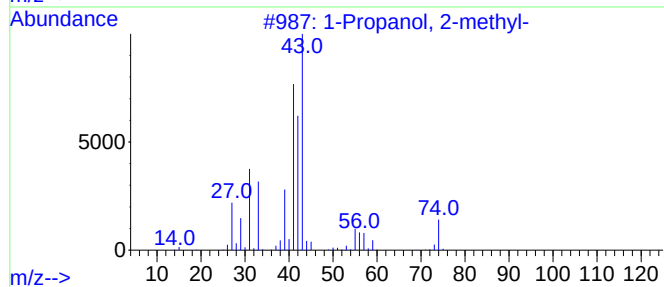
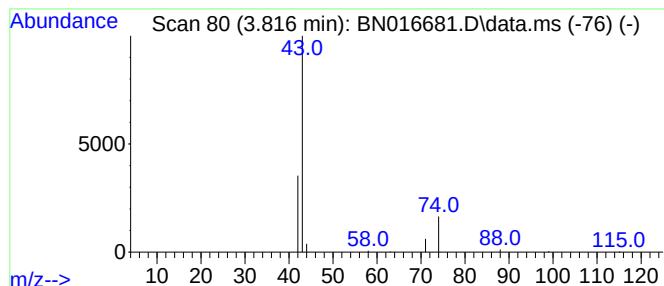
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Propanol, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.816	0.16 ng	42397	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
2			2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	5
3			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4
4			Hydrogen isocyanate	43	CHNO	000075-13-8	3
5			Acetic acid, hydrazide	74	C2H6N2O	001068-57-1	3



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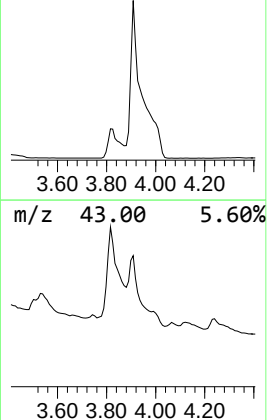
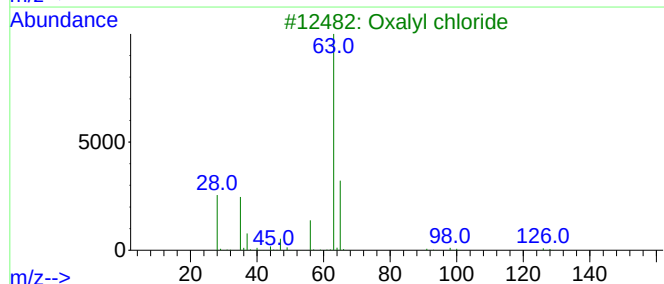
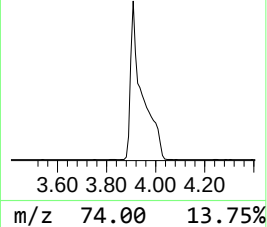
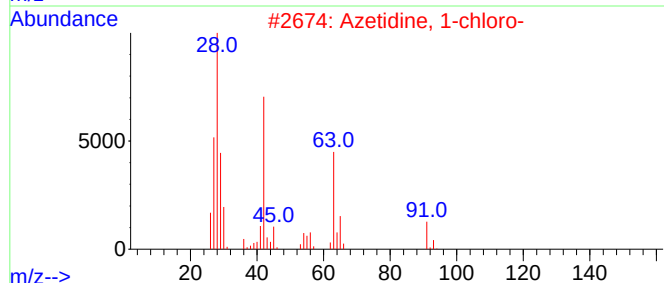
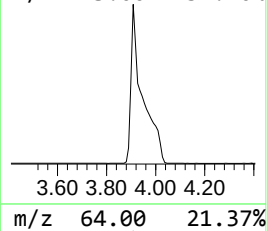
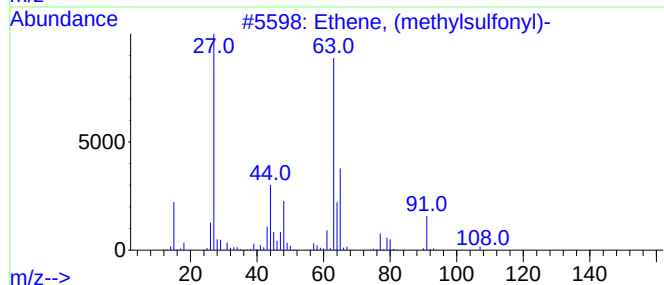
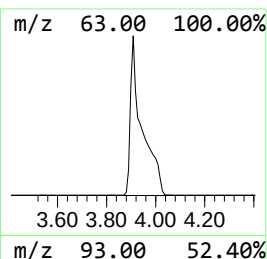
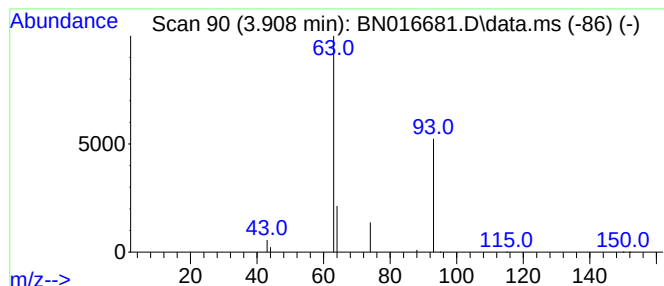
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethene, (methylsulfonyl)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.908	1.29 ng	348807	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	2
2			Azetidine, 1-chloro-	91	C3H6ClN	032115-53-0	2
3			Oxalyl chloride	126	C2Cl2O2	000079-37-8	1
4			Ethene, trifluoro-	82	C2HF3	000359-11-5	1
5			Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1



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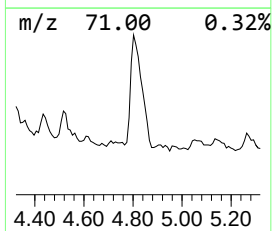
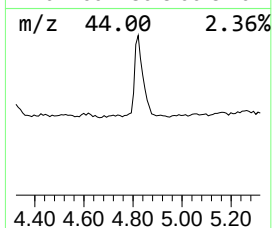
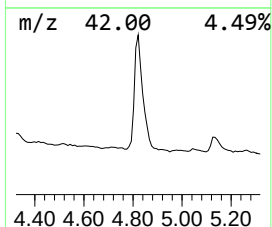
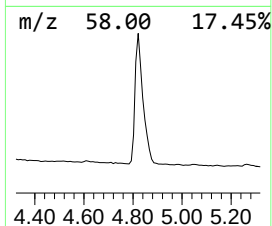
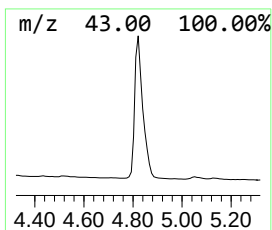
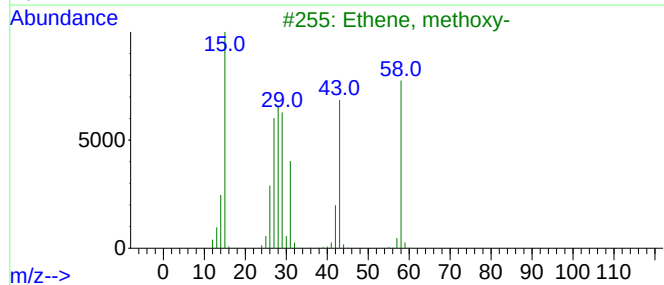
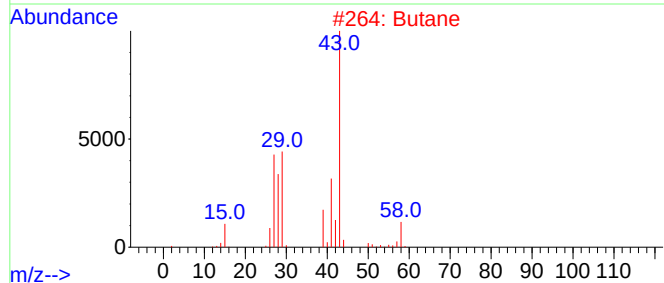
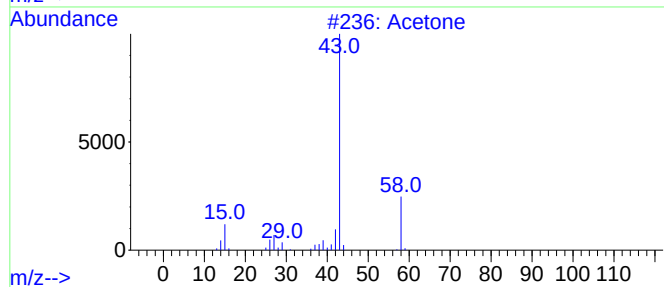
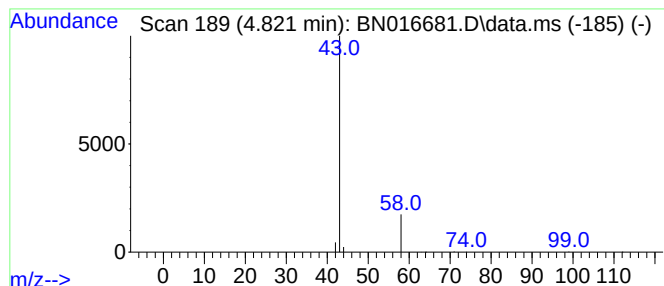
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Acetone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.821	0.40 ng	109759	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetone			58	C3H6O	000067-64-1	4
2	Butane			58	C4H10	000106-97-8	4
3	Ethene, methoxy-			58	C3H6O	000107-25-5	3
4	Diazene, dimethyl-			58	C2H6N2	000503-28-6	3
5	Hydrogen isocyanate			43	CHNO	000075-13-8	2



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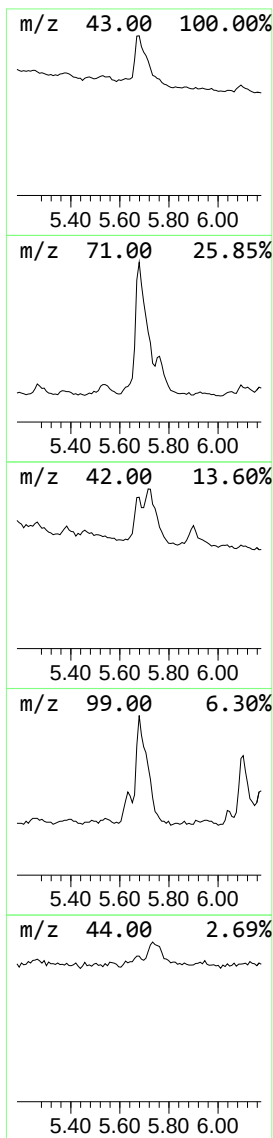
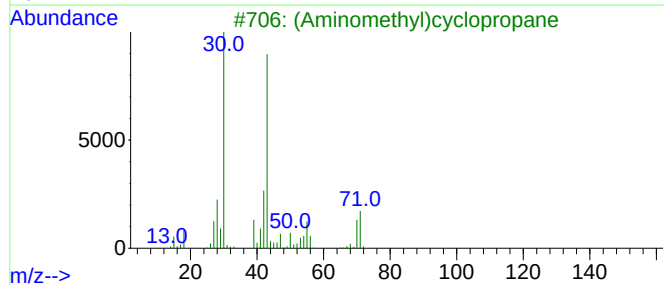
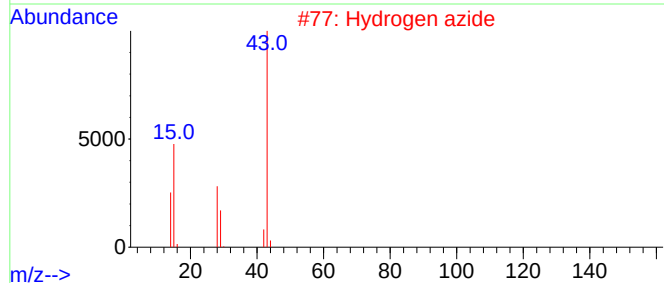
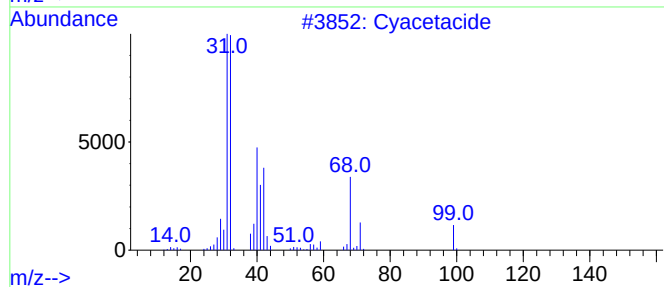
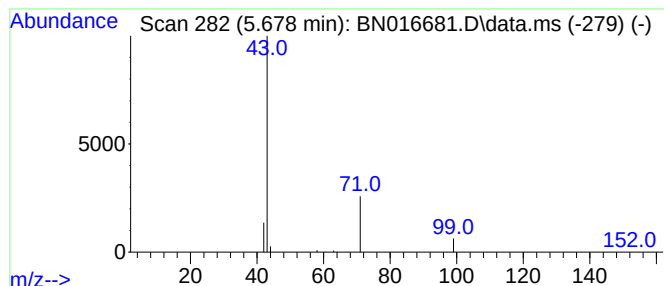
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Cyacetacide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.678	0.04 ng	11116	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyacetacide	99	C3H5N3O	000140-87-4	4
2			Hydrogen azide	43	HN3	007782-79-8	4
3			(Aminomethyl)cyclopropane	71	C4H9N	002516-47-4	3
4			1H-1,2,3,4-Tetrazol-5-amine, 1-m...	99	C2H5N5	005422-44-6	3
5			Isobutane	58	C4H10	000075-28-5	3



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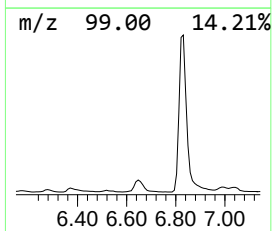
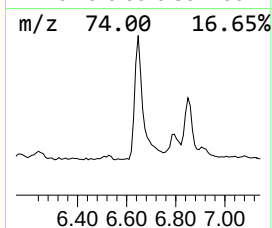
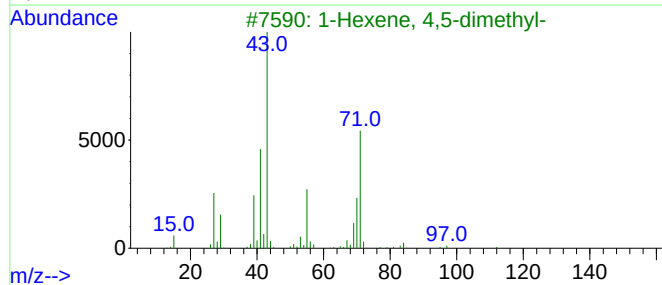
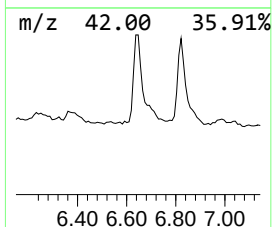
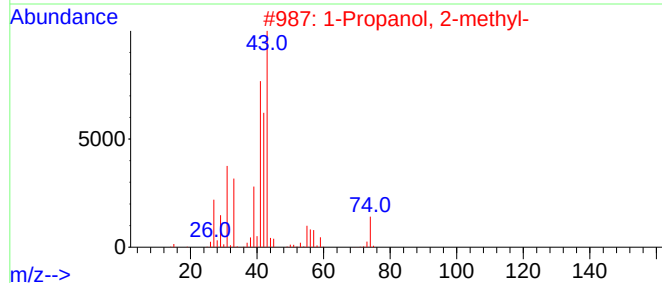
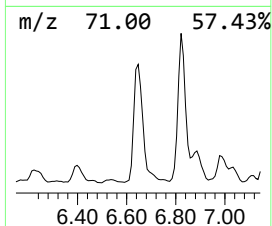
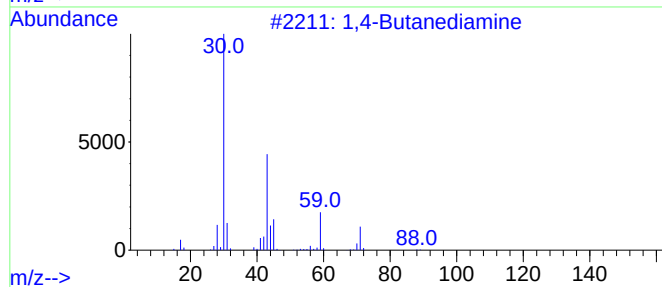
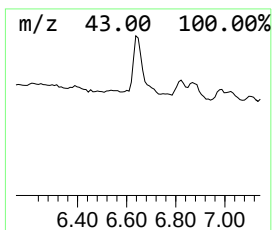
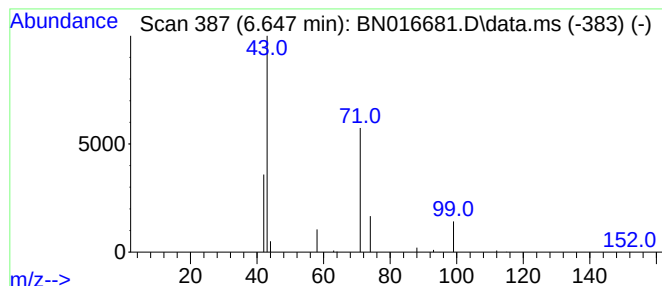
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,4-Butanediamine Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.647	0.04 ng	10968	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,4-Butanediamine	88	C4H12N2	000110-60-1	5
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	5
3			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	5
4			2-Propanone, 1-hydroxy-	74	C3H6O2	000116-09-6	4
5			Acetic acid, methyl ester	74	C3H6O2	000079-20-9	4



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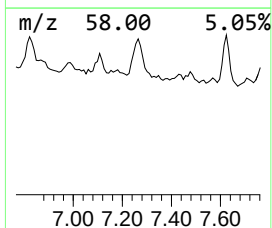
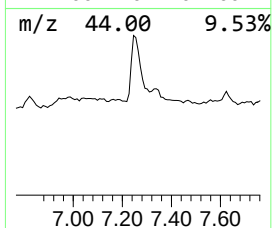
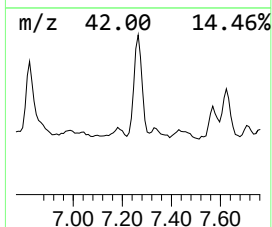
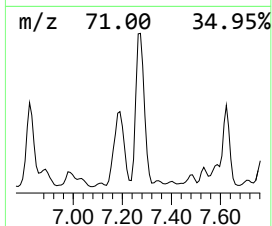
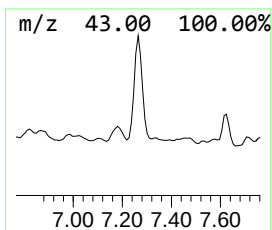
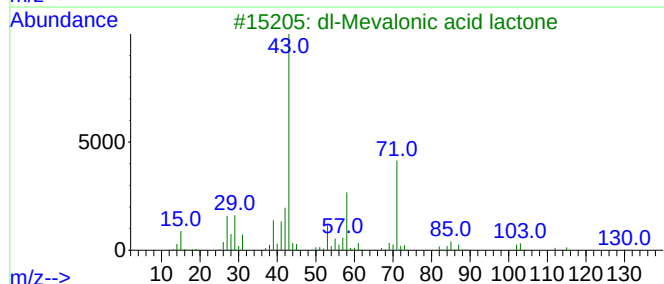
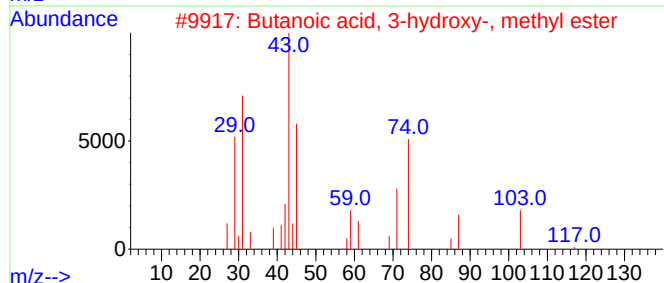
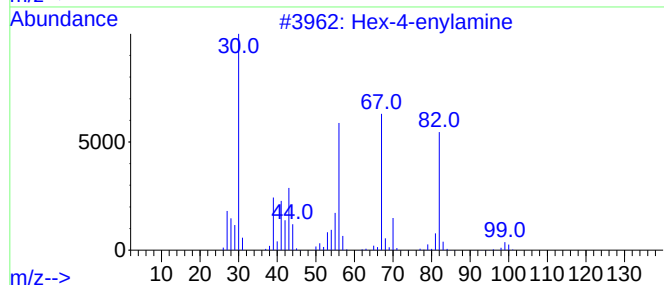
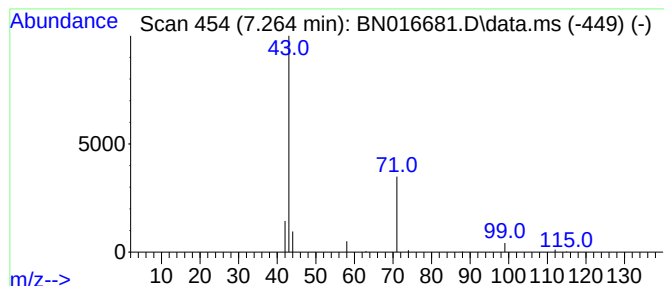
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hex-4-enylamine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.264	0.08 ng	22404	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hex-4-enylamine	99	C6H13N	055108-01-5	5
2			Butanoic acid, 3-hydroxy-, methy...	118	C5H10O3	001487-49-6	4
3			dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	4
4			Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	4
5			1-Butanol	74	C4H10O	000071-36-3	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016681.D
Acq On : 02 Oct 2021 21:21
Operator : CG/JU
Sample : M3829-24
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE123D2-20210918

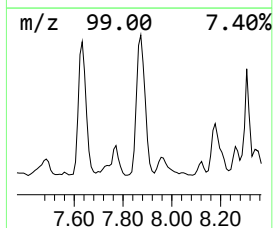
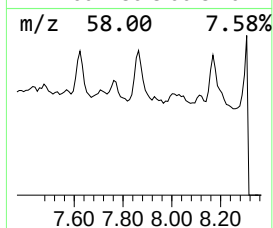
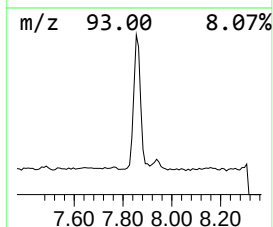
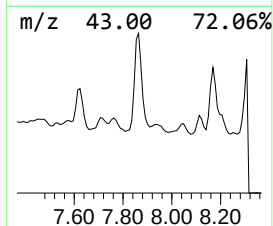
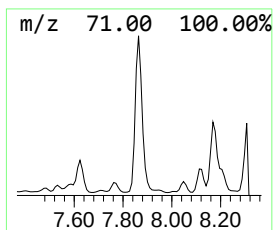
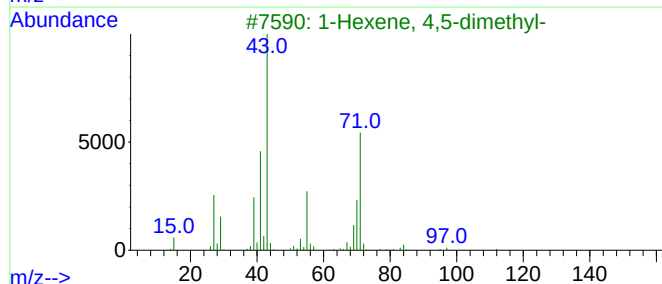
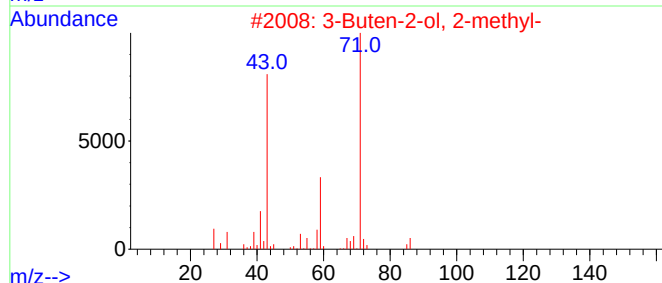
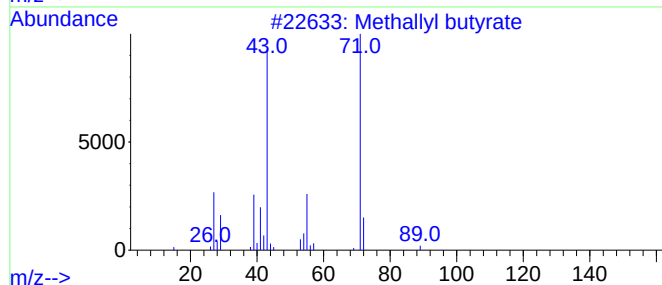
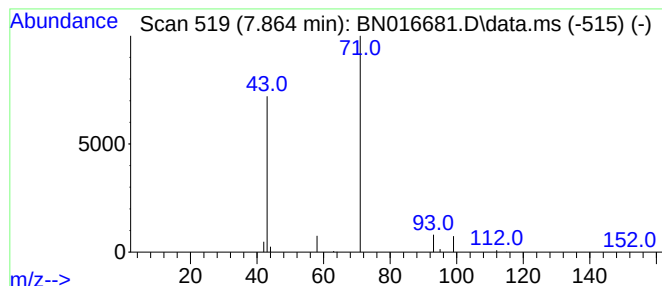
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Methallyl butyrate Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.864	0.09 ng	24060	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methallyl butyrate	142	C8H14O2	1000428-83-8	4
2			3-Buten-2-ol, 2-methyl-	86	C5H10O	000115-18-4	4
3			1-Hexene, 4,5-dimethyl-	112	C8H16	016106-59-5	4
4			Propanoic acid, 2-methyl-, anhyd...	158	C8H14O3	000097-72-3	4
5			3-Penten-2-ol	86	C5H10O	001569-50-2	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016681.D
Acq On : 02 Oct 2021 21:21
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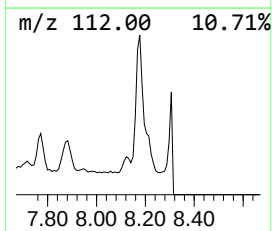
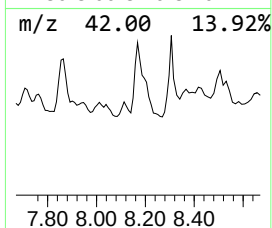
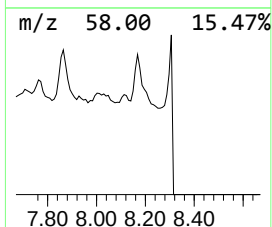
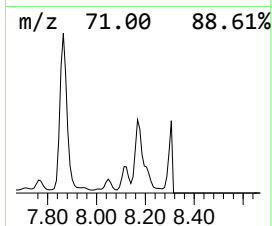
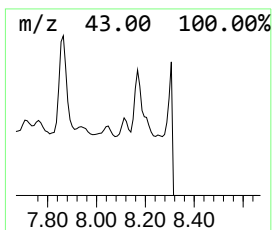
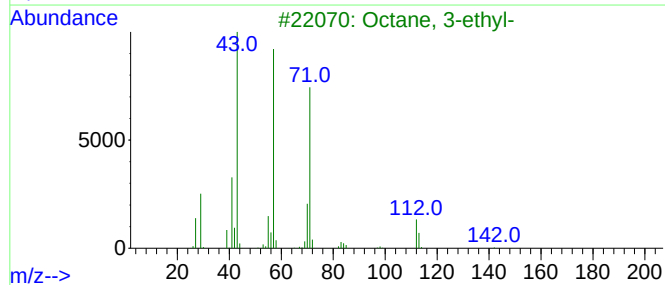
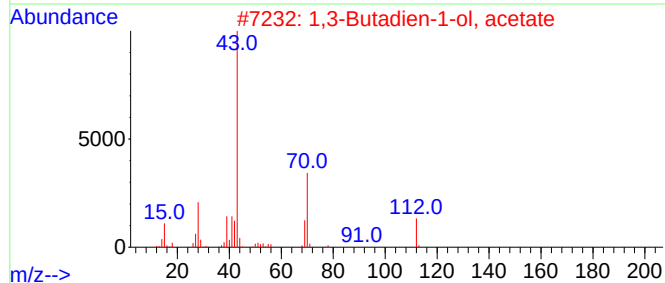
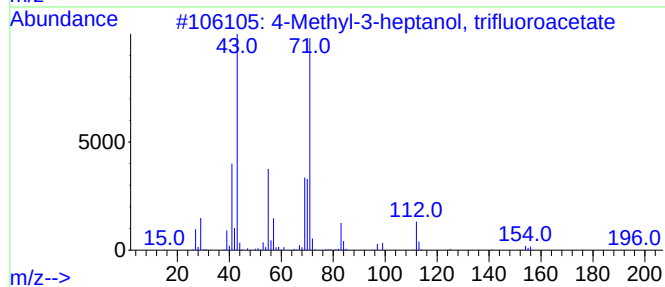
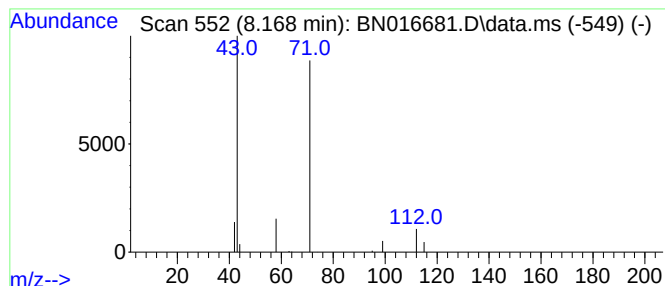
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 4-Methyl-3-heptanol, triflu... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.168	0.07 ng	20249	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Methyl-3-heptanol, trifluoroac...	226	C10H17F3O2	1000365-51-8	40
2			1,3-Butadien-1-ol, acetate	112	C6H8O2	001515-76-0	9
3			Octane, 3-ethyl-	142	C10H22	005881-17-4	9
4			Decane, 4-methyl-	156	C11H24	002847-72-5	9
5			Butane	58	C4H10	000106-97-8	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016681.D
Acq On : 02 Oct 2021 21:21
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Misc :
ALS Vial : 49 Sample Multiplier: 1

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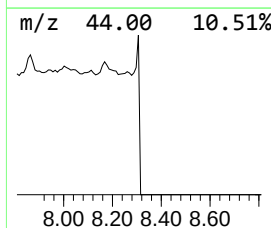
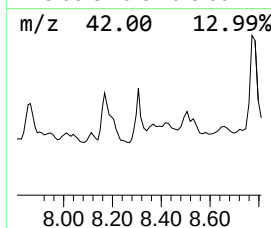
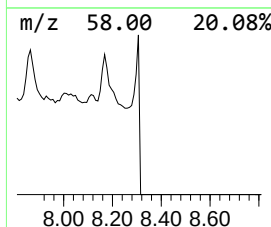
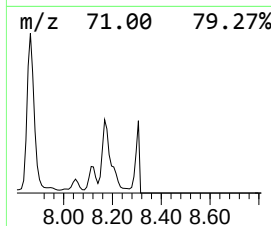
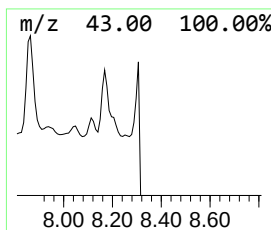
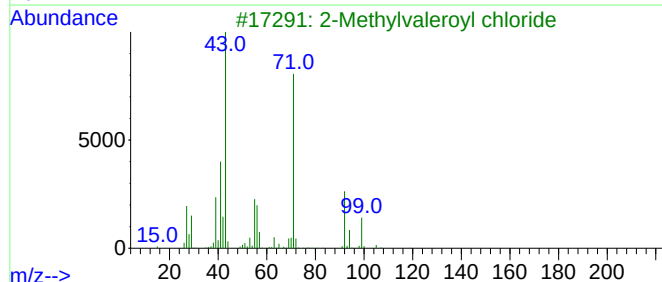
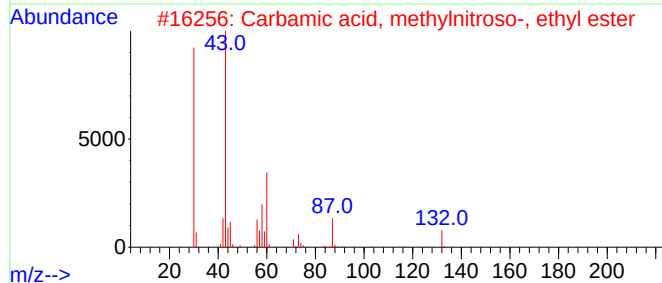
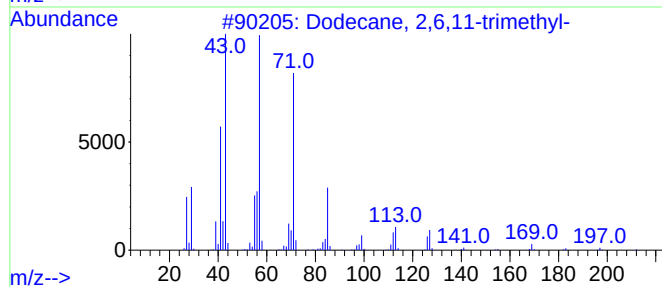
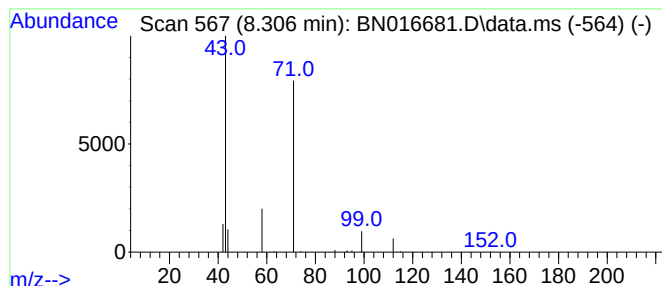
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Dodecane, 2,6,11-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.306	0.05 ng	13553	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	38
2			Carbamic acid, methylnitroso-, e...	132	C4H8N2O3	000615-53-2	9
3			2-Methylvaleroyl chloride	134	C6H11ClO	005238-27-7	9
4			Propionic acid, 2,2-dichloro-, p...	212	C8H14Cl2O2	017640-08-3	9
5			dl-Mevalonic acid lactone	130	C6H10O3	000674-26-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016681.D
Acq On : 02 Oct 2021 21:21
Operator : CG/JU
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Misc :
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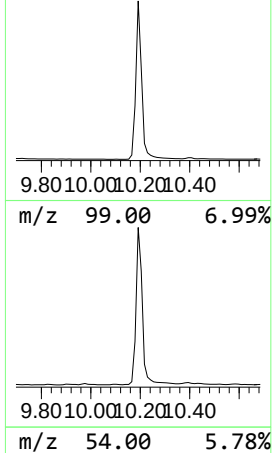
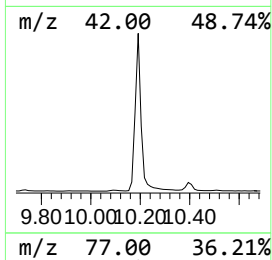
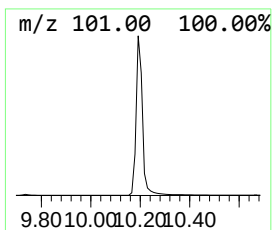
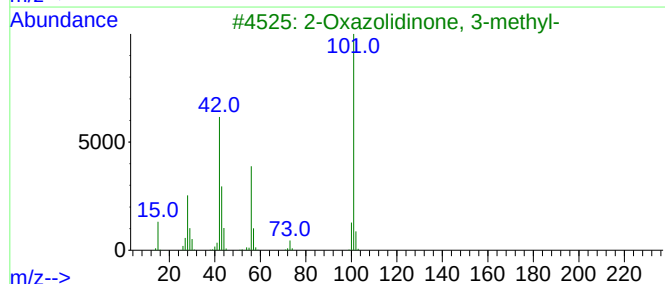
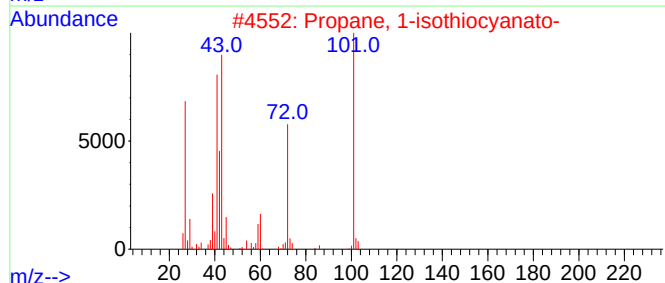
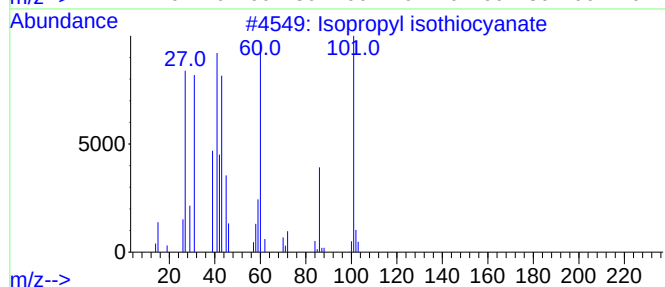
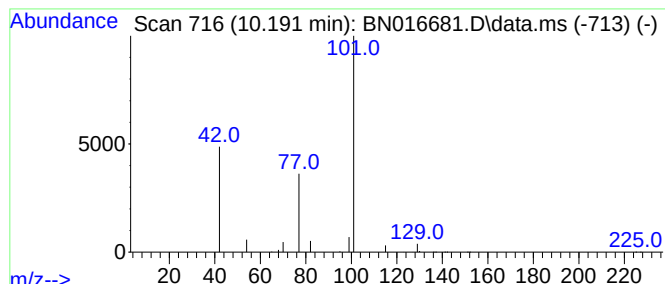
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Isopropyl isothiocyanate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.191	0.54 ng	258956	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl isothiocyanate	101	C4H7NS	002253-73-8	5
2			Propane, 1-isothiocyanato-	101	C4H7NS	000628-30-8	5
3			2-Oxazolidinone, 3-methyl-	101	C4H7N02	019836-78-3	5
4			3H-1,2,4-Triazole-3-thione, 1,2-...	101	C2H3N3S	003179-31-5	5
5			3-Aminopropionitrile	70	C3H6N2	000151-18-8	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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Operator : CG/JU
Sample : M3829-24
Misc :
ALS Vial : 49 Sample Multiplier: 1

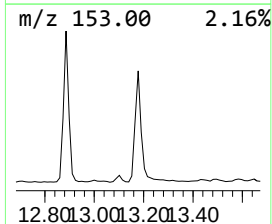
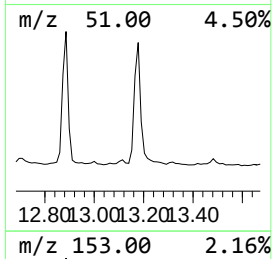
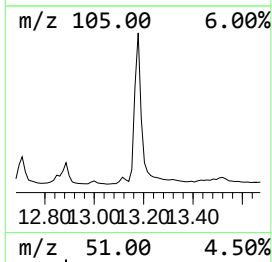
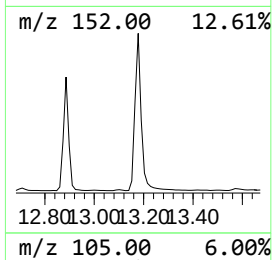
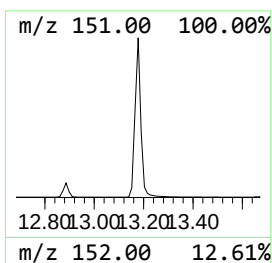
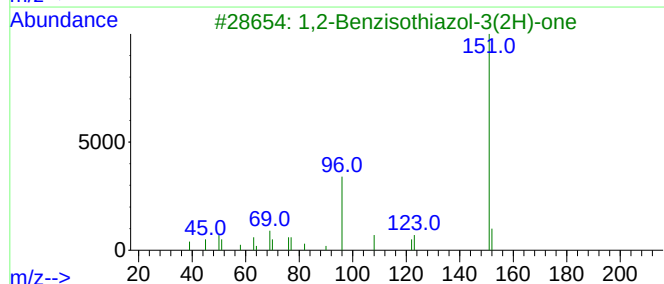
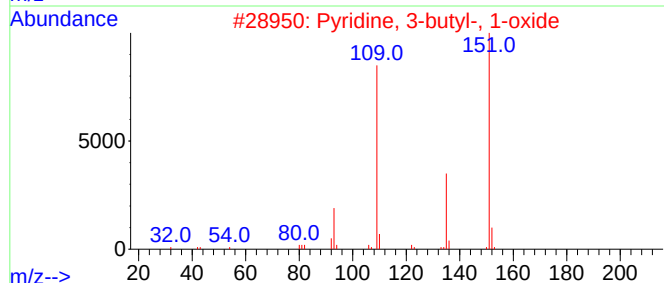
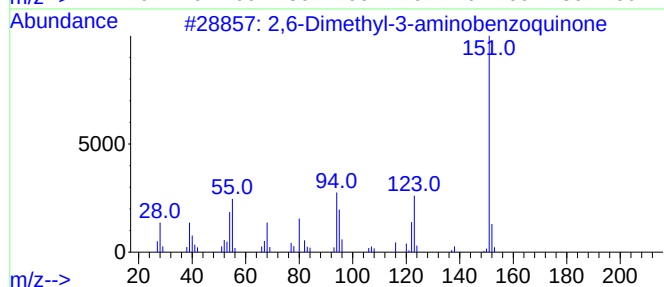
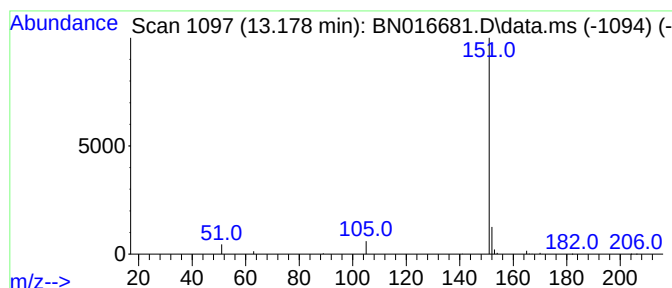
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 2,6-Dimethyl-3-aminobenzoqu... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.178	0.16 ng	81912	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	2,6-Dimethyl-3-aminobenzoquinone		151	C8H9NO2	090005-56-4	7
2	Pyridine, 3-butyl-, 1-oxide		151	C9H13NO	031396-33-5	7
3	1,2-Benzisothiazol-3(2H)-one		151	C7H5NOS	002634-33-5	7
4	7-Methyl-7H-pyrazolo(3,4-d)-v-tr...		151	C5H5N5O	018213-76-8	7
5	Carbamic acid, phenyl-, methyl e...		151	C8H9NO2	002603-10-3	7



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016681.D
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ALS Vial : 49 Sample Multiplier: 1

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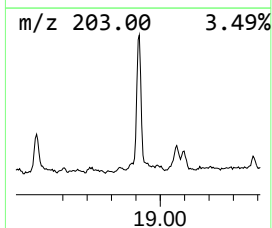
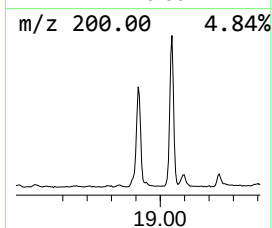
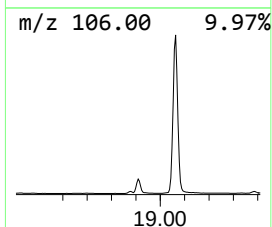
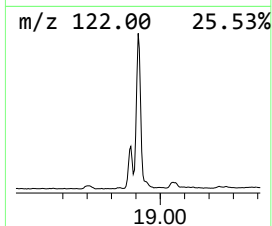
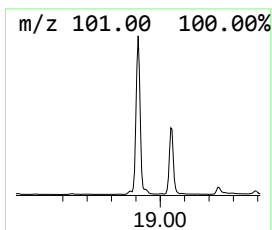
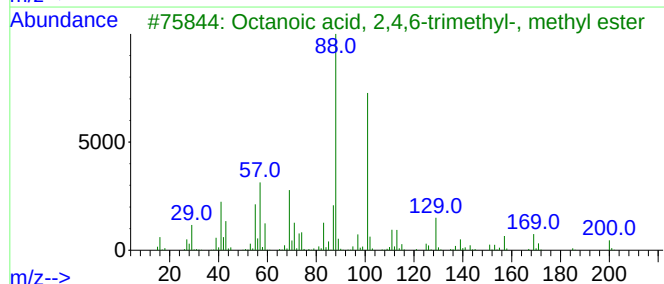
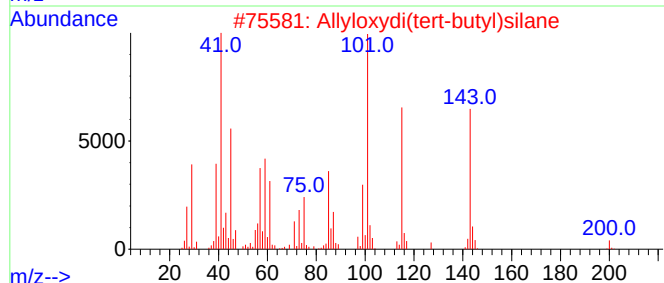
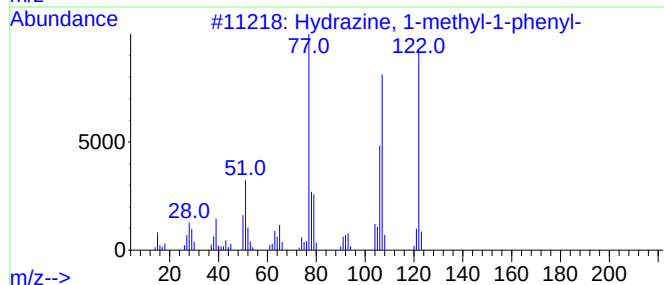
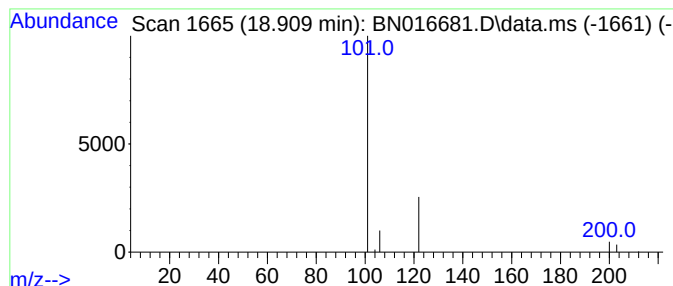
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Hydrazine, 1-methyl-1-phenyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.909	0.06 ng	26409	Phenanthrene-d10	17.018

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrazine, 1-methyl-1-phenyl-	122	C7H10N2	000618-40-6	4
2			Allyloxydi(tert-butyl)silane	200	C11H24OSi	1000279-09-4	4
3			Octanoic acid, 2,4,6-trimethyl-,...	200	C12H24O2	054984-07-5	4
4			Decanoic acid, ethyl ester	200	C12H24O2	000110-38-3	3
5			2-Aminocyclohex-1-ene-1-carbonit...	122	C7H10N2	015595-71-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016681.D
Acq On : 02 Oct 2021 21:21
Operator : CG/JU
Sample : M3829-24
Misc :
ALS Vial : 49 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
RE123D2-20210918

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol, 2-m...	3.816	0.2	ng	42397	1	7.642	108416	0.4
Ethene, (methyl...	3.908	1.3	ng	348807	1	7.642	108416	0.4
Acetone	4.821	0.4	ng	109759	1	7.642	108416	0.4
Cyacetacide	5.678	0.0	ng	11116	1	7.642	108416	0.4
1,4-Butanediamine	6.647	0.0	ng	10968	1	7.642	108416	0.4
Hex-4-enylamine	7.264	0.1	ng	22404	1	7.642	108416	0.4
Methallyl butyrate	7.864	0.1	ng	24060	1	7.642	108416	0.4
4-Methyl-3-hept...	8.168	0.1	ng	20249	1	7.642	108416	0.4
Dodecane, 2,6,1...	8.306	0.1	ng	13553	1	7.642	108416	0.4
Isopropyl isoth...	10.191	0.5	ng	258956	2	10.407	190084	0.4
2,6-Dimethyl-3-...	13.178	0.2	ng	81912	3	14.269	201262	0.4
Hydrazine, 1-me...	18.909	0.1	ng	26409	4	17.018	163843	0.4